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Technical Memorandum 33-676

*Optical Properties of Thin Gold Films Applied
to Schottky Barrier Solar Cells*

Yea-Chuan M. Yeh

(NASA-CR-137981) OPTICAL PROPERTIES OF
THIN GOLD FILMS APPLIED TO SCHOTTKY
BARRIER SOLAR CELLS (Jet Propulsion Lab.)

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PREFACE

The work described in this report was performed by the Guidance and Control Division of the Jet Propulsion Laboratory.

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ABSTRACT

The Schottky barrier solar cell is considered a possible candidate for converting solar to electrical energy both for space and terrestrial applications. Knowledge of the optical constants of the ultrathin metal film used in the cell is essential for analyzing and designing higher efficiency Schottky barrier cells. In this work, the optical constants of 7.5-nm (75-Å) gold films on gallium arsenide have been obtained. In addition, the absolute collection efficiency of Schottky barrier solar cells has been determined from measured spectral response and optical constants of the gold film.

I. INTRODUCTION

To optimize the performance of the Schottky barrier solar cell, knowledge of the role of light transmission through the thin metal film that forms the barrier is needed. Past studies of the Schottky barrier solar cell and the antireflection (A-R) coating have not fully taken into account the quasi-continuous or aggregated structure of the metal film. Because of this structure, the values of the complex index of refraction N are quite different from bulk values. The value N ($N = n - jk$), where n and k are the refractive index and extinction coefficient respectively, has been shown to depend on the wavelength, metal thickness, rate of deposition, method of deposition, and temperature and surface properties of the substrate (Refs. 1 through 9). The previous workers did not specify sufficient numbers of parameters that were required to characterize the optical property of thin metal films. In our study, the determination of the optical constants was made with thin films whose thickness as well as the conditions of their preparation are well defined.

In this article, results of an investigation of the optical constants of thin gold (Au) films on gallium arsenide (GaAs) substrates, produced by E-gun deposition, are presented. The results include: (1) the complex index of refraction, (2) transmission, reflection, and absorption, and (3) refractive index and thickness of the A-R coating requirements for Au-GaAs Schottky barrier solar cells.

II. THEORY

A. REFLECTION, TRANSMISSION, AND ABSORPTION OF LIGHT WAVES

For an isotropic medium, electro-magnetic waves are governed by Maxwell's equations:

$$\text{div } \vec{D} = \epsilon \text{ div } \vec{E} = \rho$$

$$\text{div } \vec{B} = \mu \text{ div } \vec{H} = 0$$

$$\text{curl } \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$$

$$\text{curl } \vec{H} = \sigma \vec{E} + \epsilon \frac{\partial \vec{E}}{\partial t}$$

where the symbols bear their usual meaning, and the International System of Units (MKS) are used. For a medium with no net charge, these relations lead to wave equations that describe the propagation of an electromagnetic wave.

$$\mu\epsilon \frac{\partial^2 \vec{E}}{\partial t^2} + \mu\sigma \frac{\partial \vec{E}}{\partial t} = \nabla^2 \vec{E}$$

$$\mu\epsilon \frac{\partial^2 \vec{H}}{\partial t^2} + \mu\sigma \frac{\partial \vec{H}}{\partial t} = \nabla^2 \vec{H}$$

Let us consider that a plane wave travels in the direction perpendicular to the film plane (positive Z direction). Since the tangential components of both the electric and the magnetic vectors must be continuous at the boundaries, the recurrence relation in matrix form (Ref. 2) is:

$$\begin{bmatrix} E_{m-1}^+ \\ E_{m-1}^- \end{bmatrix} = \frac{1}{t_m} \begin{bmatrix} \exp(j\delta_{m-1}) & r_m \exp(j\delta_{m-1}) \\ r_m \exp(-j\delta_{m-1}) & \exp(-j\delta_{m-1}) \end{bmatrix} \begin{bmatrix} E_m^+ \\ E_m^- \end{bmatrix}$$

where E_{m-1}^+ , E_{m-1}^- are the electric field intensity vectors in the $m-1$ layer at the interface between the m and $m-1$ layer. The superscript $+$ or $-$ indicates positive or negative Z direction, respectively. All other parameters in the matrix can be expressed in terms of the measurable parameters of the m th layer N_m (the complex index of refraction), d_m (the thickness), and λ (the wavelength in vacuum). Thus

$$r_m = \frac{N_{m-1} - N_m}{N_{m-1} + N_m}$$

$$t_m = \frac{2N_{m-1}}{N_{m-1} + N_m}$$

$$\delta_m = \frac{2\pi N_m}{\lambda} d_m$$

Then, by applying the above recurrence relation for a system with double layer films on an absorbing substrate, the percentage power reflected from the air-film interface R_2 (Fig. 1) can be expressed as a function of λ , N_m , and d_m . Since the expression is very lengthy, new symbols are introduced to express R_2 by

$$R_2(\lambda, N_m, d_m) = \frac{t_{13}^2 + u_{13}^2}{p_{13} + q_{13}}, \quad m = 0, 1, 2, 3 \quad (1)$$

where t_{13} , u_{13} , p_{13} , and q_{13} are defined as:

$$t_{13} = t_{12}p_3 - u_{12}q_3 + v_{12}t_3 - w_{12}u_3 \quad (1a)$$

$$u_{13} = u_{12}p_3 + t_{12}q_3 + w_{12}t_3 + v_{12}u_3 \quad (1b)$$

$$p_{13} = p_{12}p_3 - q_{12}q_3 + r_{12}t_3 - s_{12}u_3 \quad (1c)$$

$$q_{13} = q_{12}p_3 + p_{12}q_3 + s_{12}t_3 + r_{12}u_3 \quad (1d)$$

Part of the new symbols introduced in the above expressions are further defined as:

$$p_m = \exp(\alpha_{m-1}) \cos \gamma_{m-1}$$

$$q_m = \exp(\alpha_{m-1}) \sin \gamma_{m-1}$$

$$t_m = \exp(-\alpha_{m-1}) (g_{m-1} \cos \gamma_{m-1} + h_m \sin \gamma_{m-1})$$

$$u_m = \exp(-\alpha_{m-1}) (h_m \cos \gamma_{m-1} - g_m \sin \gamma_{m-1})$$

$$r_2 = \exp(\alpha_1) (g_2 \cos \gamma_1 - h_2 \sin \gamma_1)$$

$$s_2 = \exp(\alpha_1) (h_2 \cos \gamma_1 + g_2 \sin \gamma_1)$$

$$v_2 = \exp(-\alpha_1) \cos \gamma_1$$

$$w_2 = -\exp(-\alpha_1) \sin \gamma_1$$

$$r_{12} = r_2 + g_1 v_2 - h_1 w_2$$

$$s_{12} = s_2 + h_1 v_2 + g_1 w_2$$

$$v_{12} = v_2 + g_1 r_2 - h_1 s_2$$

$$w_{12} = w_2 + h_1 r_2 + g_1 s_2$$

where

$$\alpha_m = \frac{2\pi}{\lambda} k_m d_m$$

$$\gamma_m = \frac{2\pi}{\lambda} n_m d_m$$

$$g_m = \frac{n_{m-1}^2 - n_m^2 + k_{m-1}^2 - k_m^2}{(n_{m-1} + n_m)^2 + (k_{m-1} + k_m)^2}$$

$$h_m = \frac{2(n_{m-1}k_m - n_mk_{m-1})}{(n_{m-1} + n_m)^2 + (k_{m-1} + k_m)^2}$$

The remaining new symbols introduced in Eqs. (1a through 1d) are defined as follows:

$$t_{12} = t_2 + g_1 p_2 - h_1 q_2$$

$$u_{12} = u_2 + h_1 p_2 + g_1 q_2$$

$$p_{12} = p_2 + q_1 t_2 - h_1 u_2$$

$$q_{12} = q_2 + h_1 t_2 + g_1 u_2$$

The fractional power transmitted through the interface of the film and the substrate can also be found as:

$$T_2(\lambda, N_m, d_m) = \frac{n_3}{n_0} \times \frac{\ell_{13}^2 + o_{13}^2}{p_{13}^2 + q_{13}^2}, \quad m = 0, 1, 2, 3 \quad (2)$$

where

$$\ell_{13} = (1 + g_1)(1 + g_2)(1 + g_3) - h_2 h_3(1 + g_1)$$

$$- h_3 h_1(1 + g_2) - h_1 h_2(1 + g_3)$$

$$o_{13} = h_1(1 + g_2)(1 + g_3) + h_2(1 + g_3)(1 + g_1)$$

$$+ h_3(1 + g_1)(1 + g_2) - h_1 h_2 h_3$$

The fractional power absorption A_2 can be easily derived as:

$$A_2(\lambda, N_m, d_m) = 1 - R_2 - T_2, \quad m = 0, 1, 2, 3 \quad (3)$$

Equations (1), (2), and (3) are the basic equations that were used in the calculation of power reflection, transmission, and absorption.

B. REQUIREMENTS FOR A-R COATING

The surface impedance is the ratio of the tangential components of the electric field to the magnetic field intensity at the surface of consideration. By using the recurrent relation, the surface impedance can be obtained. Then, by an impedance matching concept, the index of refraction n as well as the thickness t of the optimum A-R coating for an absorbing film on an absorbing substrate are derived by Wolter (Refs. 10 and 11) as:

$$n(\lambda, N_m, d_m) = \left[n_0 \frac{V^2}{U - n_0} + U \right]^{1/2}, \quad m = 0, 2, 3 \quad (4)$$

$$t(\lambda, N_m, d_m) = \frac{\lambda}{2\pi n} \tan^{-1} \left(\frac{n}{n_0} \times \frac{U - n_0}{V} \right), \quad m = 0, 2, 3 \quad (5)$$

where $U(\lambda, N_m, d_m)$ and $V(\lambda, N_m, d_m)$, respectively, are the real and the imaginary part of $G(\lambda, N_m, d_m)$, where G is defined as

$$G = U - jV = \frac{1 - A}{1 + A}$$

where

$$A = \frac{(N_0 - N_2)(N_2 + N_3) \exp(\gamma_2) + (N_0 + N_2)(N_2 - N_3) \exp(-\gamma_2)}{(N_0 + N_2)(N_2 + N_3) \exp(\gamma_2) + (N_0 - N_2)(N_2 - N_3) \exp(-\gamma_2)}$$

and N_0 , N_2 , and N_3 are the index of refraction of the air, the absorbing film and the substrate, respectively.

Equations (4) and (5) are the basic equations that were used in the calculation of the A-R coating parameters.

III. EXPERIMENT

A. EXPERIMENTAL SETUP FOR REFLECTION MEASUREMENTS

The basic experiment for power reflection measurements is shown in Fig. 2. The setup consists of a Spectra Physics Model 164 ion (krypton or argon) laser, or a Spectra Physics Model 370 tunable dye laser (optically pumped by the argon laser). These lasers give a variety of wavelengths from the near UV to near IR. The laser beam is directed through a Spectra Physics Model 336 multiwavelength beam expanding and collimating telescope and then onto the sample under study. The incident and reflected power was measured by a United Detector Technology Model 21A power meter. The angle between the incident and reflected light beam from the target was approximately 2 deg, assuring that the error introduced by assuming normal incidence is negligible. The laser had a stability of better than $\pm 0.5\%$ over a 10-h period.

B. SAMPLE PREPARATION AND MEASUREMENTS

The single-crystal GaAs substrate was first lapped with 1000-grid grinding compound and then chemically polished with PA solution (30% H_2O_2 : 30% NH_4OH = 700:1) to remove the work damage and to obtain a mirror-finished surface. Immediately after the chemical polish, the surface was rinsed with deionized water and dried by a jet of microscopically clean Freon-12 gas to avoid any surface contamination. The sample was then promptly placed into an oil-diffusion pump system equipped with a liquid-nitrogen cold trap. After a pressure of $1.33 \times 10^{-5} \text{ N/m}^2$ (10^{-7} torr) was reached, gold was evaporated by E-gun and deposited on the sample. The rate of deposition and final thickness of the gold film on the sample was controlled by a Kronos Model ADS-200 digital thickness monitor system. For all experimental data presented here, the purity of gold used was better than 99.99%, and the substrate temperature was kept at room temperature.

The measurements were carried out at wavelengths of 457.9, 514.5, 580, 647.1, and 752.5 nm. The laser beam was expanded to 5 mm to

minimize any error introduced by surface irregularities on the sample. Individual measurements were repeated many times for statistical purposes, and measured reflection values have an accuracy of $\pm 1\%$.

IV. CALCULATIONS

A. CALCULATION OF n AND k

Since only the absolute value of the complex reflection R_2 in Eq. (1) was measured at a given wavelength at normal incidence, it was not possible to uniquely determine the two unknowns n and k . In the following calculations, the functional dependence of n on values of λ measured by Krautkrämer (Ref. 3) is assumed to be valid. The functional dependence of n rather than k was selected for determining N because a small change in k results in large changes in the reflection.

The values of n and k extrapolated from the experimental data of Krautkrämer (Ref. 3) were used as initial trial values in Eq. (1). The values of n and k were then varied by fixed increments at each wavelength. Thus, many pairs of n and k that gave the same calculated reflection which matched the experimental value, were obtained at each wavelength. By comparing the calculated values of n with those obtained by Krautkrämer for their functional dependence on λ , unique pairs of n and k were determined. The results are shown in Fig. 3.

B. VERIFICATION

To verify that the results for n and k obtained above are correct, the spectral response of the solar cell was measured. By inserting into Eqs. (1) and (2) the extrapolated values of n and k for gold obtained from Fig. 3, and those values of n and k for gallium arsenide obtained from Ref. 12, the fractional power transmission, reflection as well as absorption were calculated. The results with 7.5-nm (75-Å) gold film are shown in Fig. 4, in a wavelength range from 0.4 μm to 0.9 μm . The measured spectral response of the Au-GaAs Schottky barrier solar cell is shown in Fig. 5 (lower curve). After correcting for the calculated transmission, the net spectral response (defined as the ratio of the number of electron-hole pairs contributing to the external photo-current, to the number of photons

penetrating through the gold film) is shown by the upper curve in Fig. 4. Note that, before the correction was made, the collection efficiency dropped at shorter wavelength. However, after correction was made, the collection efficiency increased at the shorter wavelength as expected from the theory (Ref. 13). This finding supports the correctness of n and k values obtained in this work.

In addition, from the data of Krautkrämer (Ref. 3), the complex index of refraction of gold film as a function of film thickness at a wavelength of $0.6\ \mu\text{m}$ is plotted in Fig. 6. Our data (indicated by cross marks), which was transferred from Fig. 3 for a 7.5-nm gold film at $0.6\ \mu\text{m}$ wavelength, agreed with those of Krautkrämer's. This serves as an additional verification of the data of n and k obtained in this work.

C. CALCULATION OF THE OPTIMUM A-R COATING

Inserting values of n and k obtained from Fig. 6 into Eqs. (4) and (5), both the index of refraction n and thickness of the A-R coating t were calculated. The results are shown in Fig. 7. The reflection R of the gold film on GaAs, which has been calculated by using Eq. 1 and values of n and k in Fig. 6, is also shown in Fig. 7. In addition, the light absorption A by the gold film coated with ideal antireflection coating and calculated by employing Eqs. (1), (2), and (3), is shown in Fig. 7.

V. CONCLUSION

The optical constants, n and k , of 7.5-nm gold film (on gallium arsenide) have been obtained (Fig. 3), with information sufficient to characterize the metal film; this characterization was not available previously. Accurate knowledge of the optical constants enables one to make a more complete analysis of the Schottky barrier solar cell. The technique described in previous sections is readily used to obtain optical constants of other kinds of metals with various thicknesses.

It was found that the optimum A-R coating required for Schottky barrier cells depends greatly upon the thickness of gold film (Fig. 7). On the other hand, the A-R coating for junction cells is uniquely determined by the optical property of the semiconductor. For example, the parameters of

the optimum A-R coating for a gallium arsenide junction cell can be found at zero thickness in Fig. 7. The influence of optical properties of metal films on light transmission is very important, and therefore, the optical constants of the thin metal film are indeed needed for predicting accurately the optimum A-R coating as well as the optimum solar cell performance.

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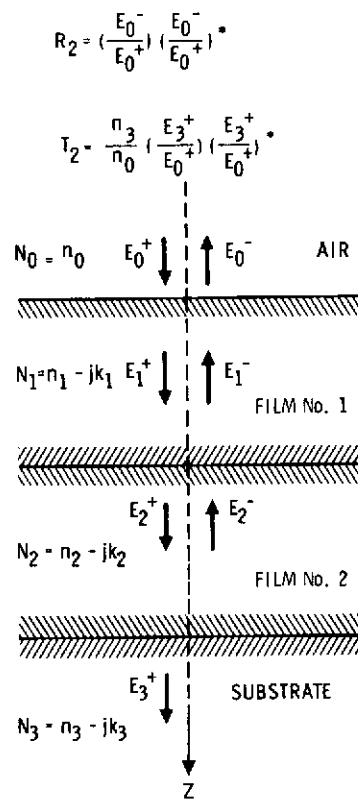


Fig. 1. Model diagram for double-layer films on an absorbing substrate

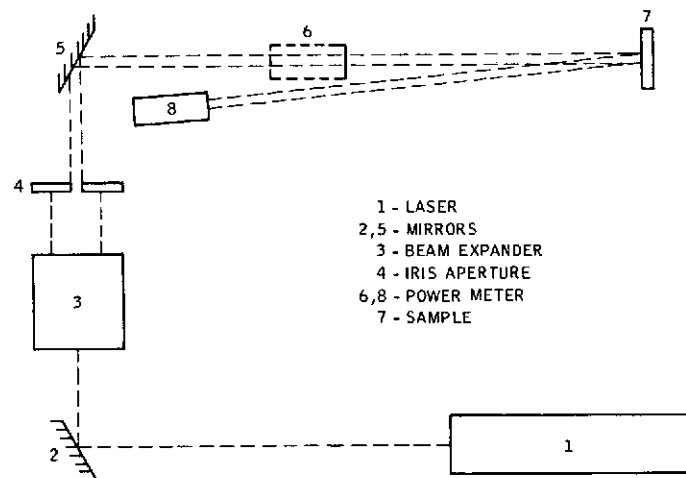


Fig. 2. Experimental setup for power reflection measurement

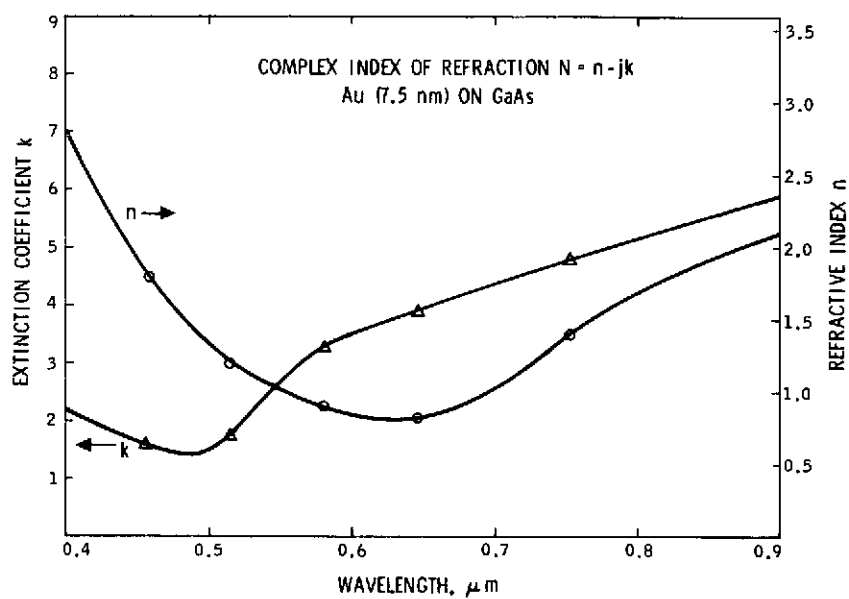


Fig. 3. Wavelength dependence of complex index of refraction

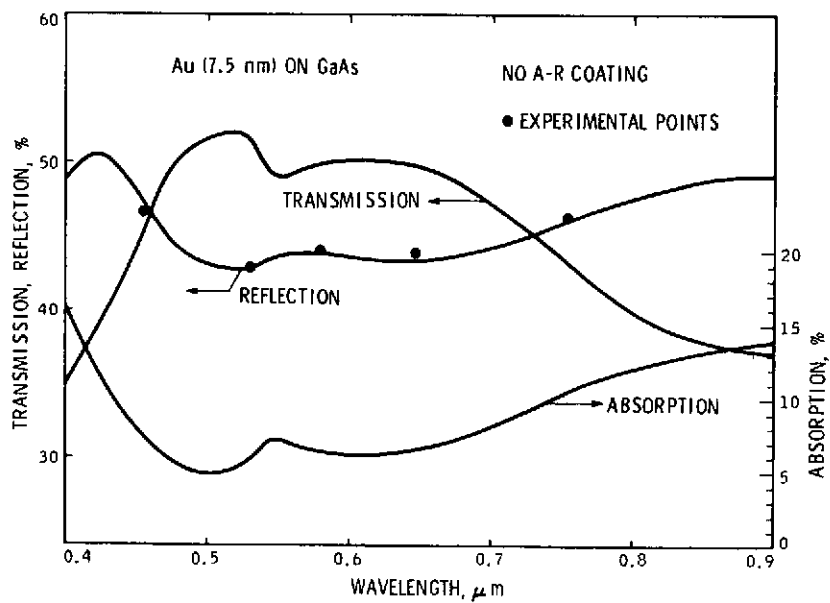


Fig. 4. Wavelength dependence of transmission, reflection, and absorption

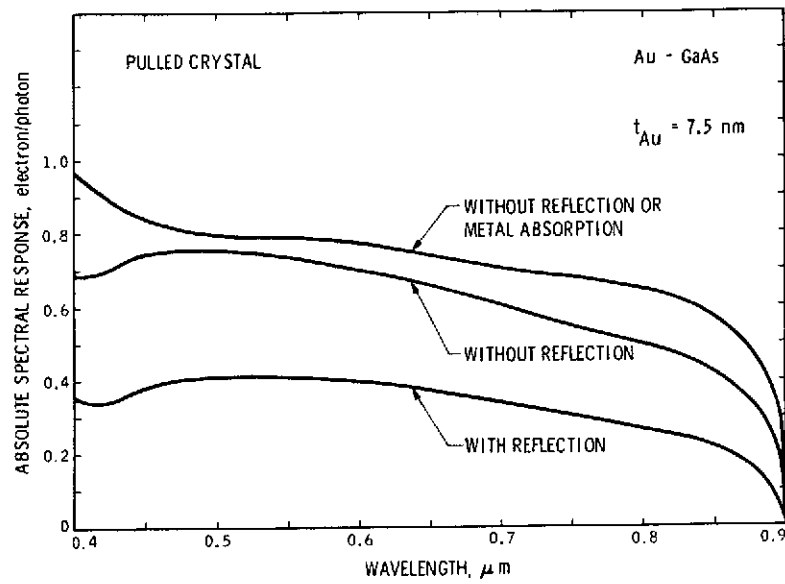


Fig. 5. Absolute spectral response of Au-GaAs solar cells

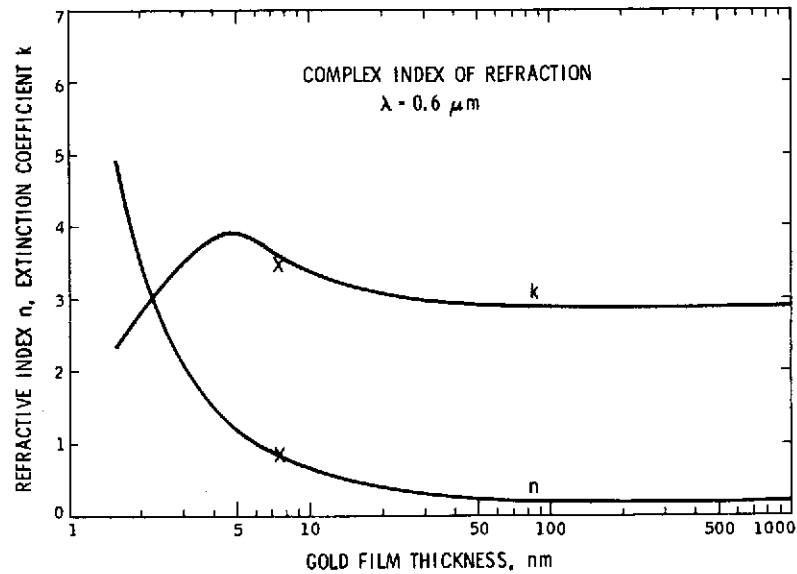


Fig. 6. Thickness dependence of the complex index of refraction

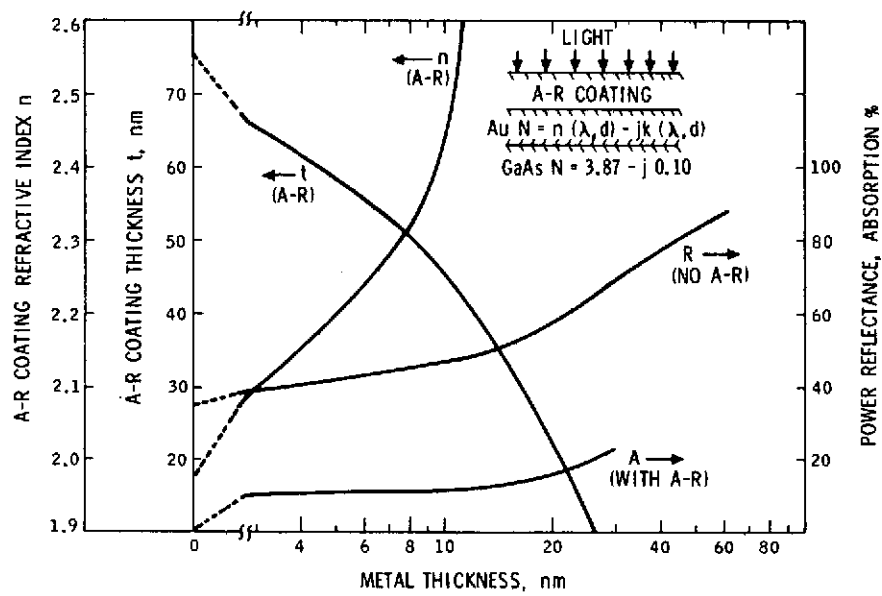


Fig. 7. Dependence of optimum A-R coating on metal thickness